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A PRODUCT VERSION OF A VARIABLE METRIC METHOD AND ITS CONVERGEN--ETC(U)

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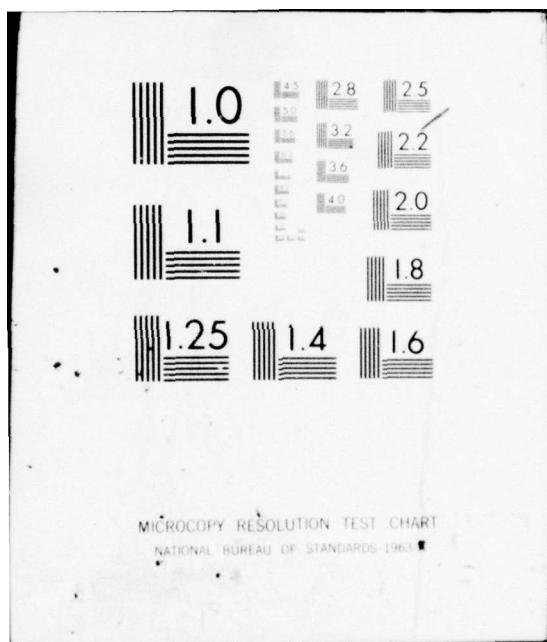
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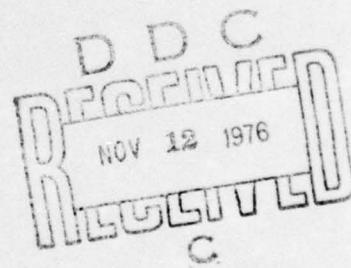
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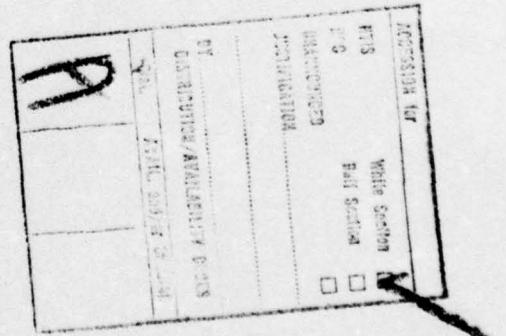
ABSTRACT

An algorithm is described which uses a product representation of the matrix  $H_j$  approximating the inverse Hessian matrix of the function to be minimized. It is shown that the algorithm generates the same sequence of points as the Broyden-Fletcher-Goldfarb-Shanno- method. Using a simple relation between the traces of the matrices  $H_j$  and  $H_{j+1}$  corresponding to two consecutive points  $x_j$  and  $x_{j+1}$  the superlinear convergence of the algorithm is established.

AMS(MOS) Classification No. 90C30

Key Words: Nonlinear programming, unconstrained minimization, variable metric methods, superlinear convergence.

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A PRODUCT VERSION OF A VARIABLE METRIC METHOD  
AND ITS CONVERGENCE PROPERTIES

Klaus Ritter

1. Introduction.

Various kinds of variable metric methods have been used effectively in the unconstrained minimization of a function of several variables. Their main feature is the use of rank one or two corrections to the matrix  $H$  which represents an approximation to the inverse Hessian matrix of the function to be minimized. Recently Brodlie, Gourlay and Greenstadt [1] and Davidon [3] used a representation of  $H$  as a product  $CC'$ . They showed that a rank two correction to  $H$  reduces to a rank one correction to  $C$ .

In this paper an algorithm is described which uses a simple rank one update formula for the matrix  $C$ . It is shown that the algorithm gives a product representation of the matrix  $H$  used in the Broyden-Fletcher-Goldfarb-Shanno-method [2], [4], [5], [6]. Under appropriate assumptions, the sequence generated by the algorithm converges superlinearly.

2. Formulation of the problem and notation.

Let  $x \in E^n$  and let  $F(x)$  be a real-valued function. We assume that  $F(x)$  is twice continuously differentiable and denote the gradient and the Hessian matrix of  $F(x)$  at a point  $x_i$  by  $g_i = \nabla F(x_i)$  and  $G_i = G(x_i)$ , respectively. A prime is used for the transpose of a vector or a matrix.

We consider the problem of determining a  $z$  such that

$$(2.1) \quad F(z) < F(x) \quad \text{for all } x \neq z.$$

It is assumed that there are positive numbers  $\mu$ ,  $\eta$  and  $L$  such that

$$(2.2) \quad \mu \|x\|^2 \leq x'G(y)x \leq \eta \|x\|^2 \quad \text{for all } x, y \in E^n$$

and

$$\|G(x) - G(y)\| \leq L\|x-y\| \quad \text{for all } x, y \in E^n.$$

Assumption (2.2) implies that  $F(x)$  is uniformly convex and that there is a unique  $z$  with property (2.1). It is determined by the condition  $\nabla F(z) = 0$ . For later use we state two more well-known results which are immediate consequences of (2.2):

$$(2.3) \quad \|G(y)\| \leq \eta, \quad \|(G(y))^{-1}\| \leq \mu^{-1} \quad \text{for all } y \in E^n$$

$$(2.4) \quad \text{There are numbers } \gamma_1 > 0 \text{ and } \gamma_2 > 0 \text{ such that for all } x \in E^n$$
$$\gamma_1 \|\nabla F(x)\| \leq \|x-z\| \leq \gamma_2 \|\nabla F(x)\|.$$

### 3. The Algorithm.

In a variable metric method at a given point  $x_j$ , the search direction  $s_j$  is determined by multiplying the gradient  $g_j = \nabla F(x_j)$  by an appropriate matrix  $H_j$ , i.e.,

$$s_j = H_j g_j,$$

where  $H_j$  is an approximation to the inverse Hessian matrix of  $F(x)$  at  $x_j$ .

With a suitable step size  $\sigma_j$  a new point

$$x_{j+1} = x_j - \sigma_j s_j$$

is computed. If  $g_{j+1} = \nabla F(x_{j+1}) \neq 0$ , the matrix  $H_{j+1}$  is determined from  $H_j$  in such a way that

$$(3.1) \quad H_{j+1}(g_j - g_{j+1}) = \sigma_j s_j.$$

The various variable metric methods differ in the updating procedure which is used to compute  $H_{j+1}$  from  $H_j$  subject to (3.1). In many methods

$H_j$  is a symmetric positive definite matrix and  $H_{j+1}$  is obtained by adding two symmetric matrices of rank one to  $H_j$ .

Any symmetric positive definite matrix  $H_j$  can be written in the form

$$(3.2) \quad H_j = C_j C_j^T ,$$

where  $C_j$  is a nonsingular matrix. Instead of adding a rank two correction matrix to  $H_j$  we can add a rank one matrix  $uv^T$  to  $C_j$  and represent  $H_{j+1}$  in the form

$$(3.3) \quad H_{j+1} = (I + uv^T)C_j C_j^T (I + vu^T)$$

where the vectors  $u$  and  $v$  are determined in such a way that (3.1) is satisfied and  $H_{j+1}$  is nonsingular.

Brodlie, Gourlay and Greenstadt [1] and more recently Davidon [3] have investigated representations of the form (3.2) and (3.3) of  $H_j$  and  $H_{j+1}$ , respectively, for some variable metric methods. In the following we shall

describe an algorithm which uses a very simple update procedure of the form

(3.3). It will be shown that this algorithm produces the same matrix  $H_{j+1}$  as the Broyden-Fletcher-Goldfarb-Shanno-method; see [2], [4], [5], [6].

We describe a general cycle of the algorithm. At the beginning of the  $j$ th cycle the following data is available:  $C_j = (c_{1j}, \dots, c_{nj})$ ,  $x_j$ ,  $g_j$  and  $\alpha_{ij} = c_{ij}^T g_j$ ,  $i = 1, \dots, n$ . For the initial cycle any nonsingular  $(n \times n)$ -matrix  $C_0$  can be used.

Step 1: Computation of the direction of descent  $s_j$ .

Set

$$s_j = \sum_{i=1}^n \alpha_{ij} c_{ij}$$

Step 2: Computation of the step size  $\sigma_j$ .

Compute  $\sigma_j$  such that

$$F(x_j - \sigma_j s_j) = \min\{F(x_j - \sigma s_j) \mid \sigma \geq 0\}$$

Set

$$x_{j+1} = x_j - \sigma_j s_j$$

and compute  $g_{j+1}$ . If  $g_{j+1} = 0$  stop, otherwise go to Step 3.

Step 3: Computation of  $C_{j+1}$ .

Compute

$$\beta_{ij} = C_{ij}' g_{j+1}, \quad i = 1, \dots, n,$$

$$\gamma_j = s_j' g_j, \quad \delta_j = s_j' g_{j+1},$$

$$\omega_{ij} = \frac{1}{\gamma_j - \delta_j} [(\sqrt{(1 - \delta_j \gamma_j^{-1}) \sigma_j} - 1) \alpha_{ij} + \beta_{ij}], \quad i = 1, \dots, n.$$

Set

$$c_{i,j+1} = c_{ij} + \omega_{ij} s_j \quad i = 1, \dots, n.$$

$$\alpha_{i,j+1} = \beta_{ij} + \omega_{ij} \delta_j$$

Replace  $j$  with  $j+1$  and go to Step 1.

Remark:

In Step 1, the search direction  $s_j$  is determined by

$$s_j = C_j C_j' g_j.$$

In Step 2, we assume that  $\sigma_j$  is the optimal step size. This assumption is

made in order to avoid some technical difficulties in the convergence proofs.

The algorithm also works with an approximation to the optimal step size which after a finite number of steps can be set equal to 1. This will be shown in a much more general context in a subsequent paper. In Step 3,  $C_{j+1}$  is obtained by simply adding a multiple of  $s_j$  to each row of  $C_j$ . Obviously

$\delta_j = 0$ , if  $\sigma_j$  is the optimal step size.

In the following theorem it will be shown that the search directions  $s_j$  generated by the above algorithm are identical with the search directions used in the Broyden-Fletcher-Goldfarb-Shanno-method.

Theorem 1:

Let  $c_{1j}, \dots, c_{nj}$ ,  $\sigma_j$ ,  $s_j$ ,  $g_j$  and  $g_{j+1}$  be defined by the algorithm.

Set

$$C_j = (c_{1j}, \dots, c_{nj}), \quad H_j = C_j C_j^T,$$

$$p_j = \frac{s_j}{\|s_j\|}, \quad d_j = \frac{g_j - g_{j+1}}{\|\sigma_j s_j\|}$$

and

$$H_{j+1} = H_j + \frac{d_j^T p_j + d_j^T H_j d_j}{(d_j^T p_j)^2} p_j p_j^T - \frac{p_j d_j^T H_j + H_j d_j^T p_j}{d_j^T p_j}.$$

Then

$$s_{j+1} = C_{j+1} C_{j+1}^T g_{j+1}$$

and

$$H_{j+1} = C_{j+1} C_{j+1}^T.$$

Proof:

The first assertion follows immediately from Steps 1 and 3 of the algorithm since

$$c_{1j+1}^T g_{j+1} = (c_{1j} + \omega_{1j} s_j)^T g_{j+1} = \beta_{1j} + \omega_{1j} \delta_j = \alpha_{1,j+1}.$$

In order to prove the second statement we observe that

$$\begin{aligned} c_{1j+1}^T - c_{1j}^T &= ((\sqrt{(1 - \delta_j \gamma_j^{-1}) \sigma_j} - 1) \frac{c_{1j}^T g_j}{s_j^T (g_j - g_{j+1})} + \frac{c_{1j}^T g_{j+1}}{s_j^T (g_j - g_{j+1})}) s_j^T \\ &= (\sqrt{(1 - \delta_j \gamma_j^{-1}) \sigma_j} \frac{c_{1j}^T g_j}{p_j^T (g_j - g_{j+1})} - \frac{c_{1j}^T (g_j - g_{j+1})}{p_j^T (g_j - g_{j+1})}) p_j. \end{aligned}$$

Since

$$\begin{aligned} \sqrt{(1 - \delta_j \gamma_j^{-1})\sigma_j} \frac{1}{p_j'(g_j - g_{j+1})} &= \sqrt{\frac{\sigma_j p_j'(g_j - g_{j+1})}{p_j' g_j}} \frac{1}{p_j'(g_j - g_{j+1})} \\ &= \sqrt{\frac{\sigma_j}{p_j' g_j p_j'(g_j - g_{j+1})}} \end{aligned}$$

it follows that

$$C'_{j+1} - C'_j = \left( \frac{1}{\sqrt{p_j' g_j d_j' p_j}} \frac{C'_j g_j}{\sqrt{\|s_j\|}} \right) - \frac{1}{d_j' p_j} C'_j d_j p'_j .$$

Therefore

$$\begin{aligned} C_{j+1} C'_{j+1} &= C_j C'_j + (C_{j+1} - C_j) C'_j + C_j (C''_{j+1} - C'_j) + (C_{j+1} - C_j) (C'_{j+1} - C_j) \\ &= H_j + p_j \left( \frac{1}{\sqrt{p_j' g_j d_j' p_j}} \frac{s_j}{\sqrt{\|s_j\|}} - \frac{d_j' H_j}{d_j' p_j} \right) \\ &\quad + \left( \frac{1}{\sqrt{p_j' g_j d_j' p_j}} \frac{s_j}{\sqrt{\|s_j\|}} - \frac{H_j d_j}{d_j' p_j} \right) p' \\ &\quad + p_j \left( \frac{g_j' H_j g_j}{d_j' p_j g_j' p_j \|s_j\|} - \frac{2 d_j' H_j g_j}{d_j' p_j \sqrt{p_j' g_j d_j' p_j \|s_j\|}} + \frac{d_j' H_j d_j}{(d_j' p_j)^2} \right) p'_j \\ &= H_j + \frac{d_j' p_j + d_j' H_j d_j}{(d_j' p_j)^2} p_j p'_j - \frac{p_j d_j' H_j + H_j d_j p'_j}{d_j' p_j} . \end{aligned}$$

#### 4. Convergence.

If the algorithm terminates with some  $x_j$ , then  $\nabla F(x_j) = 0$  and the assumptions on  $F(x)$  imply that  $x_j$  is the unique global minimizer of  $F(x)$ . For the remainder of the paper we shall assume that the algorithm generates an infinite sequence  $\{x_j\}$ . In order to prove that it converges to the global minimizer of  $F(x)$  we shall use the equivalence with the BFGS-Method established in Theorem 1.

First we shall write  $H_j$  as a sum of  $n$  matrices of rank one. For this purpose let

$$\rho_j = \|H_j g_j\|^{-1} \quad , \quad \lambda_j = \|H_j g_{j+1}\|^{-1}$$

and

$$H_j \rho_j g_j = p_j \quad , \quad H_j \lambda_j g_{j+1} = q_j .$$

Then  $\|p_j\| = \|q_j\| = 1$  and  $\rho_j g_j$  and  $\lambda_j g_{j+1}$  are conjugate with respect to  $H_j$  since

$$\rho_j g_j' H_j g_{j+1} = p_j' g_{j+1} = 0 .$$

Assuming that  $H_j$  is positive definite we can find vectors  $d_{3j}, \dots, d_{nj}$  such that

$$H_j d_{ij} = p_{ij} , \quad \|p_{ij}\| = 1 , \quad i = 3, \dots, n$$

and

$$\rho_j g_j, \lambda_j g_{j+1}, d_{3j}, \dots, d_{nj}$$

are conjugate with respect to  $H_j$ . Then

$$(4.1) \quad H_j = \frac{p_j p_j'}{\rho_j g_j' p_j} + \frac{q_j q_j'}{\lambda_j g_{j+1}' q_j} + \sum_{i=3}^n \frac{p_{ij} p_{ij}'}{d_{ij}' p_{ij}}$$

and

$$(4.2) \quad H_j^{-1} = \frac{\rho_j g_j g_j'}{g_j' p_j} + \frac{\lambda_j g_{j+1} g_{j+1}'}{g_{j+1}' q_j} + \sum_{i=3}^n \frac{d_{ij} d_{ij}'}{d_{ij}' p_{ij}} .$$

Using (4.1) we can easily derive a corresponding expression for  $H_{j+1}$ .

First we observe that

$$H_j d_j = \frac{H_j g_j - H_j g_{j+1}}{\|\sigma_j s_j\|} = \frac{1}{\sigma_j} p_j - q_j \frac{\|H_j g_{j+1}\|}{\|\sigma_j s_j\|}$$

implies that

$$H_{j+1} x = H_j x \quad \text{for } x \in T_j = \{x | p_j' x = q_j' x = 0\} .$$

$d_{1j}, \dots, d_{nj} \in T_j$  we have to change only the first two terms in (4.1)

in order to obtain a representation of  $H_{j+1}$ , i.e., we have to determine two vectors in the span of  $g_j$  and  $g_{j+1}$  which are conjugate with respect to  $H_{j+1}$ .

We have

$$(4.3) \quad d_j \in \text{span} \{g_j, g_{j+1}\}, \quad H_{j+1} d_j = p_j, \quad \text{and} \quad d_j^T H_{j+1} d_j = d_j^T p_j > 0.$$

Furthermore,

$$(4.4) \quad g_{j+1}^T H_{j+1} d_j = g_{j+1}^T p_j = 0.$$

Thus  $g_{j+1}$  and  $d_j$  are conjugate with respect to  $H_{j+1}$ . By the definition of  $H_{j+1}$

$$(4.5) \quad \begin{aligned} H_{j+1} g_{j+1} &= H_j g_{j+1} - p_j - \frac{d_j^T H_j g_{j+1}}{d_j^T p_j} \\ &= (g_j - \alpha_j p_j) \|H_j g_{j+1}\|, \quad \alpha_j = \frac{d_j^T g_j}{d_j^T p_j} \end{aligned}$$

and

$$(4.6) \quad g_{j+1}^T H_{j+1} g_{j+1} = g_{j+1}^T q_j \|H_j g_{j+1}\| > 0.$$

With

$$\rho_{j+1} = \|H_{j+1} g_{j+1}\|^{-1}, \quad H_{j+1} \rho_{j+1} g_{j+1} = p_{j+1}$$

it follows from (4.1)-(4.6), that  $H_{j+1}$  and  $H_{j+1}^{-1}$  are positive definite and

can be written in the form

$$(4.7) \quad H_{j+1} = \frac{p_{j+1} p_{j+1}^T}{\rho_{j+1} g_{j+1}^T p_{j+1}} + \frac{p_j p_j^T}{d_j^T p_j} + \sum_{i=3}^n \frac{p_{ij} p_{ij}^T}{d_{ij}^T p_{ij}}$$

and

$$(4.8) \quad H_{j+1}^{-1} = \frac{\rho_{j+1} g_{j+1} g_{j+1}^T}{g_{j+1}^T p_{j+1}} + \frac{d_j d_j^T}{d_j^T p_j} + \sum_{i=1}^n \frac{d_{ij} d_{ij}^T}{d_{ij}^T p_j}.$$

By the definition of  $H_{j+2}$

$$H_{j+2} x = H_{j+1} x \quad \text{for} \quad x \in T_{j+1} = \{x \mid H_{j+1} g_{j+1} = H_{j+1} g_{j+2} = 0\}.$$

Setting

$$q_{j+1} = \frac{H_{j+1} g_{j+2}}{\|H_{j+1} g_{j+2}\|}, \quad \lambda_{j+1} = \frac{1}{\|H_{j+1} g_{j+2}\|}$$

and observing that

$$p_{j+1}^T g_{j+1}^T H_{j+1} g_{j+2} = p_{j+1}^T g_{j+2} = 0$$

we can write  $H_{j+1}$  and  $H_{j+1}^{-1}$  as follows

$$(4.9) \quad H_{j+1} = \frac{p_{j+1} p'_{j+1}}{p_{j+1} g'_{j+1} p_{j+1}} + \frac{q_{j+1} q'_{j+1}}{\lambda_{j+1} g'_{j+1} q_{j+1}} + \sum_{i=3}^n \frac{p_{i,j+1} p'_{i,j+1}}{d'_{i,j+1} p_{i,j+1}}$$

and

$$(4.10) \quad H_{j+1}^{-1} = \frac{p_{j+1} g_{j+1} g_{j+1}}{g'_{j+1} p_{j+1}} + \frac{\lambda_{j+1} g_{j+2} g'_{j+2}}{g'_{j+2} q_{j+1}} + \sum_{i=3}^n \frac{d_{i,j+1} d'_{i,j+1}}{d'_{i,j+1} p_{i,j+1}}$$

where  $d_{3,j+1}, \dots, d_{n,j+1}$  are vectors in  $T_{j+1}$  with

$$d'_{i,j+1} H_{j+1} d_{k,j+1} = 0, \quad i \neq k, \quad i, k = 3, \dots, n,$$

$$\|H_{j+1} d_{i,j+1}\| = 1, \quad H_{j+1} d_{i,j+1} = p_{i,j+1}, \quad i = 3, \dots, n.$$

This representation is completely analogous to (4.1) and (4.2) and can be used to derive a representation of  $H_{j+2}$  as a sum of  $n$  matrices of rank one.

In the following convergence proof we shall use a simple argument involving the trace of the matrices  $H_j$  and  $H_{j+1}$ . By definition, the trace of a square matrix  $M$ , denoted by  $\text{tr}(M)$ , is the sum of the diagonal elements of  $M$ .

From (4.1) and (4.2) we have

$$(4.11) \quad \text{tr}(H_j) = \text{tr}\left(\frac{p_j p'_j}{p_j g'_j p_j}\right) + \text{tr}\left(\frac{q_j q'_j}{\lambda_j g'_{j+1} q_j}\right) + \sum_{i=3}^n \text{tr}\left(\frac{p_{ij} p'_{ij}}{d'_{ij} p_{ij}}\right)$$

$$= \frac{1}{p_j g'_j p_j} + \frac{1}{\lambda_j g'_{j+1} q_j} + \sum_{i=3}^n \frac{1}{d'_{ij} p_{ij}}$$

and

$$(4.12) \quad \text{tr}(H_j^{-1}) = \frac{p_j \|g_j\|^2}{g'_j p_j} + \frac{\lambda_j \|g_{j+1}\|^2}{g'_{j+1} q_j} + \sum_{i=3}^n \frac{\|d_{ij}\|^2}{d'_{ij} p_{ij}}.$$

Setting  $\tau_j = (1 + \lambda_j^2 \|g_{j+1}\|^2) / \lambda_j g'_{j+1} q_j$ ,  $\omega_j = (1 + \|d_j\|^2) / d_j p_j$ ,

$$(4.13) \quad \varphi_j = \tau_j + \sum_{i=3}^n \frac{1 + \|d_{ij}\|^2}{d'_{ij} p_{ij}},$$

and

$$(4.15) \quad \varphi_{j+1} = \frac{1 + \lambda_{j+1}^2 \|g_{j+2}\|^2}{\lambda_{j+1} g_{j+2}' p_{j+1}} + \sum_{i=3}^n \frac{1 + \|d_{i,j+1}\|^2}{d_{i,j+1}' p_{i,j+1}}$$

we conclude from (4.7) - (4.12) that

$$(4.16) \quad \begin{aligned} \varphi_{j+1} &= \text{tr}(H_{j+1}) - \frac{1}{\rho_{j+1} g_{j+1}' p_{j+1}} + \text{tr}(H_{j+1}^{-1}) - \frac{\rho_{j+1} \|g_{j+1}\|^2}{g_{j+1}' p_{j+1}} \\ &= \omega_j + \sum_{i=3}^n \frac{1 + \|d_{ij}\|^2}{d_{ij}' p_{ij}} \\ &= \varphi_j - \tau_j + \omega_j. \end{aligned}$$

The equality (4.16) will be used to prove that the sequence of gradients produced by the algorithm converges to zero. First we observe that  $\varphi_{j+1} > 0$  since  $H_{j+1}$  is positive definite and, therefore, all terms on the right hand side of (4.15) are positive. Secondly we shall show (Lemma 1) that, because of the assumptions on  $F(x)$ , the sequence  $\{\omega_j\}$  is bounded. This implies that there is a constant  $\gamma$  and an infinite set  $J \subset \{0, 1, 2, \dots\}$  such that

$$(4.17) \quad \tau_j \leq \gamma \quad \text{for } j \in J.$$

Using the definition of  $\tau_j$  and  $p_{j+1}$  it can easily be shown (Lemma 2) that there is  $\varepsilon > 0$  such that

$$g_{j+1}' p_{j+1} \geq \varepsilon \|g_{j+1}\| \quad \text{for } j \in J.$$

By a routine argument it follows from this that

$$\|g_{j+1}\| \rightarrow 0 \quad \text{as } j \rightarrow \infty, \quad j \in J,$$

which by the uniform convexity of  $F(x)$  implies

$$\|g_{j+1}\| \rightarrow 0 \quad \text{as } j \rightarrow \infty$$

Lemma 1.

$$\omega_j = \frac{1 + \|d_j\|^2}{d_j' p_j} \leq \frac{1 + \eta^2}{\mu} \quad \text{for all } j.$$

Proof:

By Taylor's theorem there are

$$\xi_j, \eta_j \in \{x \mid x = x_j - t(\sigma_j s_j), 0 \leq t \leq 1\}$$

such that

$$p_j^T g_{j+1} = p_j^T g_j - \sigma_j p_j^T G(\xi_j) s_j$$

and

$$d_j^T g_{j+1} = d_j^T g_j - \sigma_j d_j^T G(\eta_j) s_j.$$

Therefore,

$$(4.18) \quad d_j^T p_j = \frac{(g_j - g_{j+1})^T p_j}{\|\sigma_j s_j\|} = p_j^T G(\xi_j) p_j \geq \mu$$

and

$$(4.19) \quad \|d_j\|^2 = \frac{d_j^T (g_j - g_{j+1})}{\|\sigma_j s_j\|} = d_j^T G(\eta_j) p_j \leq \|d_j\| \|G(\eta_j)\| \leq \eta \|d_j\|.$$

Lemma 2.

For every  $\gamma > 0$  there is  $\varepsilon > 0$  such that, for all  $j$ ,

$$\tau_j = \frac{1 + \lambda_j^2 \|g_{j+1}\|^2}{\lambda_j g_{j+1}^T q_j} \leq \gamma \text{ implies } g_{j+1}^T p_{j+1} \geq \varepsilon \|g_{j+1}\|.$$

Proof:

If  $\tau_j \leq \gamma$ , then

$$\gamma \geq \frac{\|g_{j+1}\|}{g_{j+1}^T q_j} \left( \frac{1}{\lambda_j \|g_{j+1}\|} + \lambda_j \|g_{j+1}\| \right) \geq 2 \frac{\|g_{j+1}\|}{g_{j+1}^T q_j}$$

and

$$\frac{g_{j+1}^T q_j}{\|g_{j+1}\|} \geq \frac{2}{\gamma}.$$

By (4.5),

$$p_{j+1} = (q_j - \frac{d_j^T q_j}{d_j^T p_j} p_j) \|q_j - \frac{d_j^T q_j}{d_j^T p_j} p_j\|^{-1}.$$

Since, by (4.18) and (4.19),

$$\|q_j - \frac{d_j' q_j}{d_j' p_j} p\| \leq 1 + \frac{|d_j' q_j|}{d_j' p_j} \leq 1 + \frac{\|d_j\|}{d_j' p_j} \leq 1 + \frac{\eta}{\mu},$$

it follows that

$$\frac{p_{j+1}' g_{j+1}}{\|g_{j+1}\|} \geq \frac{\mu}{1+\eta} \frac{g_{j+1}' q_j}{\|g_{j+1}\|} \geq \frac{2\mu}{\gamma(1+\eta)}.$$

Theorem 2.

The sequence  $\{x_j\}$  generated by the algorithm converges to a  $z$  such that

$$F(z) < F(x) \text{ for all } x \neq z$$

and

$$\nabla F(z) = 0.$$

Proof:

By (4.17) and Lemma 1 and 2 there is  $\varepsilon > 0$  and an infinite set  $J \subset \{0, 1, 2, \dots\}$  such that

$$g_j' p_j \geq \varepsilon \|g_j\| \text{ for } j \in J.$$

Furthermore, it follows from Taylor's theorem that, for some  $\xi_j \in \{x \mid x = x_j - t(\sigma s_j), 0 \leq t \leq 1\}$ ,

$$\begin{aligned} F(x_j - \sigma s_j) - F(x_j) &= -\sigma g_j' s_j + \frac{1}{2} \sigma^2 s_j' G(\xi_j) s_j \\ &\leq -\sigma g_j' s_j + \frac{1}{2} \sigma^2 \eta \|s_j\|^2. \end{aligned}$$

Thus choosing

$$\tilde{\sigma} = \frac{g_j' s_j}{\eta \|s_j\|^2}$$

we obtain, for  $j \in J$ ,

$$\begin{aligned}
 F(x_{j+1}) - F(x_j) &\leq F(x_j - \tilde{\sigma} s_j) - F(x_j) \\
 &\leq -\frac{1}{2\eta} \frac{(g_j^T s_j)^2}{\|s_j\|^2} \\
 &\leq -\frac{\epsilon^2}{2\eta} \|g_j\|.
 \end{aligned}$$

Since  $F(x)$  is bounded from below and  $F(x_{j+1}) < F(x_j)$  for all  $j$ , it follows that

$$\|g_j\| \rightarrow 0 \text{ as } j \rightarrow \infty, \quad j \in J.$$

Let  $z$  be a cluster point of the sequence  $\{x_j, j \in J\}$ . Then  $\nabla F(z) = 0$ . By the uniform convexity of  $F(x)$ ,  $z$  is the unique global minimizer of  $F(x)$ . Since  $F(x_{j+1}) < F(x_j)$  for all  $j$ , the sequence  $\{x_j\}$  has no cluster point except  $z$ . Thus  $x_j \rightarrow z$  as  $j \rightarrow \infty$ .

##### 5. Superlinear convergence.

In order to prove that

$$\frac{\|g_{j+1}\|}{\|g_j\|} \rightarrow 0 \quad \text{as } j \rightarrow \infty$$

we shall again use the trace of the matrices  $H_j$  and  $H_{j+1}$ . The argument will be based on a modification of the formula (4.16).

By Theorem 2,  $x_j \rightarrow z$  as  $j \rightarrow \infty$ . Let  $G = G(z)$  and denote by  $G^{\frac{1}{2}}$  the square root of  $G$ . By definition  $G^{\frac{1}{2}}$  is a symmetric positive definite matrix with the property

$$G = G^{\frac{1}{2}} G^{\frac{1}{2}}.$$

We set  $G^{-\frac{1}{2}} = (G^{\frac{1}{2}})^{-1}$ . Replacing the matrices  $H_j$  and  $H_j^{-1}$  by  $G^{\frac{1}{2}} H_j G^{\frac{1}{2}}$  and  $(G^{\frac{1}{2}} H_j G^{\frac{1}{2}})^{-1} = G^{-\frac{1}{2}} H_j^{-1} G^{-\frac{1}{2}}$ ,

respectively, in the formulae (4.1), (4.2) and (4.7) - (4.16) we obtain

$$\omega_j = \frac{p_j' G p_j + d_j' G^{-1} d_j}{d_j' p_j}, \quad \tau_j = \frac{q_j' G q_j + \lambda_j^2 g_{j+1} G^{-1} g_{j+1}}{\lambda_j g_{j+1} q_j},$$

$$\varphi_j = \tau_j + \sum_{i=3}^n \frac{p_{ij}' G p_{ij} + d_{ij}' G^{-1} d_{ij}}{d_{ij}' p_{ij}}$$

and

$$(5.1) \quad \varphi_{j+1} = \zeta_j - \tau_j + \omega_j.$$

In order to prove that  $\{\|g_j\|\}$  converges superlinearly to zero we observe that by Taylor's theorem

$$\begin{aligned} \|d_j - Gp_j\| &= \left\| \left( \int_0^1 G(x_j - t \sigma_j s_j) dt - G \right) p_j \right\| \\ &\leq \sup_{0 \leq t \leq 1} \|G(x_j - t \sigma_j s_j) - G_j\| + \|G_j - G\| \\ &\leq L \|x_j - x_{j+1}\| + L \|x_j - z\| \\ &= O(\max\{\|g_j\|, \|g_{j+1}\|\}). \end{aligned}$$

Thus Lemma 3 below implies that  $\omega_j \rightarrow 2$  as  $j \rightarrow \infty$ . Since  $\varphi_j > 0$  we shall conclude from this that  $\tau_j \rightarrow 2$  as  $j \rightarrow \infty$ . Setting

$$\psi_j = \text{tr} \left( \frac{G^{\frac{1}{2}} p_j p_j' G^{\frac{1}{2}}}{p_j g_j' p_j} \right) + \text{tr} \left( \frac{\rho_j G^{-\frac{1}{2}} g_j g_j' G^{-\frac{1}{2}}}{g_j' p_j} \right)$$

we obtain from Lemma 4 that  $\psi_j \rightarrow 2$  as  $j \rightarrow \infty$  which by Lemma 5 in turn implies that  $\|g_{j+1}\| \|g_j\|^{-1} \rightarrow 0$  as  $j \rightarrow \infty$ .

Lemma 3.

Let  $x, y \in E^n$  be such that  $\|x\| = 1$  and  $y'x > 0$ . Set

$$\tau = \text{tr} \left( \frac{G^{\frac{1}{2}} x x' G^{\frac{1}{2}}}{y' x} \right) + \text{tr} \left( \frac{G^{-\frac{1}{2}} y y' G^{-\frac{1}{2}}}{y' x} \right).$$

Then

$$\tau \geq 2$$

and there is a constant  $\gamma > 0$  such that  $\tau - 2 \leq \gamma$  implies

$$y'x \geq \frac{1}{2}\mu, \quad \|Gx-y\|^2 \leq \eta(\eta+\mu)(\tau-2)$$

and  $\|Gx-y\| \leq \gamma$  implies

$$\tau-2 \leq \frac{2}{\mu^2} \|Gx-y\|^2.$$

Proof:

Set  $v = y - Gx$ . Then

$$\begin{aligned} \tau &= \frac{x'Gx + y'G^{-1}y}{y'x} = \frac{2x'Gx + 2v'x + v'G^{-1}v}{x'Gx + v'x} \\ &= 2 + \frac{v'G^{-1}v}{x'Gx + v'x} \end{aligned}$$

Thus  $\tau \geq 2$  and

$$\begin{aligned} \frac{1}{\eta} \|v\|^2 &\leq v'G^{-1}v = (\tau-2)(x'Gx + v'x) \\ &\leq (\tau-2)(\|G\| + \|v\|) \leq (\tau-2)(\eta + \|v\|) \end{aligned}$$

Therefore, we have

$$\|v\| \leq (\tau-2)\eta \left[ \frac{\eta}{\|v\|} + 1 \right]$$

which implies that for  $\tau-2$  sufficiently small  $\|v\| \leq 0.5\mu$ . Thus, for  $\gamma$  sufficiently small,

$$\|v\|^2 \leq \eta(\eta+\mu)(\tau-2)$$

and

$$y'x = x'Gx + v'x \geq \mu - \|v\| \geq 0.5\mu.$$

Finally, for  $\|Gx-y\| \leq 0.5\mu$ ,

$$\tau-2 \leq \frac{\|v\|^2 \|G^{-1}\|}{\mu - \|v\|} \leq \frac{2\|v\|^2}{\mu^2}.$$

Lemma 4.

There is a constant  $\gamma > 0$  such that, for all  $j$ ,  $\tau_j - 2 \leq \gamma$  implies

$$|\psi_{j+1} - \tau_j| = O(\max\{\sqrt{\tau_j-2}, \|g_j\|\}).$$

Proof:

By (4.5)

$$p_{j+1} = (q_j - \alpha_j p_j) \|q_j - \alpha_j p_j\|^{-1}.$$

Therefore,  $\rho_{j+1} = \lambda_{j+1} \|q_j - \alpha_j p_j\|^{-1}$  implies

$$\begin{aligned} \rho_{j+1} g'_{j+1} p_{j+1} &= \rho_{j+1} g'_{j+1} q_j \|q_j - \alpha_j p_j\|^{-1} \\ &= \lambda_{j+1} g'_{j+1} q_j \|q_j - \alpha_j p_j\|^{-2}. \end{aligned}$$

Furthermore,

$$p'_{j+1} G p_{j+1} = \|q_j - \alpha_j p_j\|^{-2} (q_j - \alpha_j p_j)' G (q_j - \alpha_j p_j)$$

and

$$\begin{aligned} \psi_{j+1} &= \frac{p'_{j+1} G p_{j+1} + \rho_{j+1}^2 g'_{j+1} G^{-1} g_{j+1}}{\rho_{j+1} g'_{j+1} p_{j+1}} \\ &= \frac{(q_j - \alpha_j p_j)' G (q_j - \alpha_j p_j) + \rho_{j+1}^2 \|q_j - \alpha_j p_j\|^2 g'_{j+1} G^{-1} g_{j+1}}{\lambda_{j+1} g'_{j+1} q_j} \\ &= \tau_j + \frac{\alpha_j^2 p'_{j+1} G p_{j+1} - 2\alpha_j q'_{j+1} G p_{j+1}}{\lambda_{j+1} g'_{j+1} q_j}. \end{aligned}$$

By definition,  $\alpha_j = d'_j q_j / d'_j p_j$  and

$$\begin{aligned} d'_j q_j &= p'_j G q_j + (d'_j - p'_j G) q_j \\ &= p'_j (\lambda_{j+1} g_{j+1}) - p'_j (\lambda_{j+1} g_{j+1} - G q_j) + (d'_j - p'_j G) q_j. \end{aligned}$$

Therefore,

$$|d'_j q_j| \leq \|\lambda_{j+1} g_{j+1} - G q_j\| + \|d'_j - G p_j\|.$$

Since,  $\|d'_j - G p_j\| = O(\max\{\|g_j\|, \|g_{j+1}\|\})$ ,  $d'_j p_j \geq \mu$  and Lemma 3 implies that for  $\gamma$  sufficiently small

$$\|\lambda_{j+1} g_{j+1} - G q_j\| = O(\sqrt{\tau_j - 2})$$

and

$$\lambda_{j+1} g_{j+1}' q_j \geq 0.5\mu$$

we have

$$\begin{aligned} |\psi_{j+1} - \tau_j| &\leq \frac{\alpha_j^2 \|G\| + 2\alpha_j \|G\|}{0.5\mu} \\ &= O(\max\{\sqrt{\tau_j - 2}, \|g_j\|, \|g_{j+1}\|\}). \end{aligned}$$

Lemma 5.

There is a constant  $\gamma > 0$  such that, for all  $j$ ,  $\psi_j - 2 \leq \gamma$

implies

$$\begin{aligned} \text{i)} \quad |\sigma_j - 1| &= O(\max\{\sqrt{\psi_j - 2}, \|g_j\|, \|g_{j+1}\|\}) \\ \text{ii)} \quad \frac{\|g_{j+1}\|}{\|g_j\|} &= O(\max\{\sqrt{\psi_j - 2}, \|g_j\|, \|g_{j+1}\|\}). \end{aligned}$$

Proof:

By Taylor's theorem there is

$$\xi_j \in \{x \mid x = x_j - t(\sigma_j s_j), 0 \leq t \leq 1\}$$

such that

$$0 = s_j' g_{j+1} = s_j' g_j - \sigma_j s_j' G(\xi_j) s_j.$$

Thus

$$(5.2) \quad \sigma_j = \frac{g_j' s_j}{s_j' G(\xi_j) s_j} = 1 - \frac{g_j' s_j - s_j' G(\xi_j) s_j}{s_j' G(\xi_j) s_j}.$$

Since with  $v_j = \rho_j g_j - G p_j$  we have

$$g_j' s_j = \left(\frac{p_j'}{\rho_j} G + \frac{v_j'}{\rho_j}\right) s_j = s_j' G s_j + v_j' s_j \|s_j\|,$$

and it follows that

$$\begin{aligned}
|\sigma_j - 1| &= \frac{s_j' G s_j + v_j' s_j \|s_j\| - s_j' G(\xi_j) s_j}{s_j' G(\xi_j) s_j} \\
&\leq \frac{s_j' (G - G(\xi_j)) s_j + \|v_j\| \|s_j\|^2}{\mu \|s_j\|^2} \\
&\leq \frac{1}{\mu} (\|G - G(\xi_j)\| + \|v_j\|) \\
&= O(\max \{\sqrt{\psi_j - 2}, \|g_j\|, \|g_{j+1}\|\}),
\end{aligned}$$

where the last equality follows from Lemma 3 and (2.4) since

$$\|G - G(\xi_j)\| \leq \|G - G_j\| + \|G_j - G(\xi_j)\| \leq L \|x_j - z\| + L \|x_{j+1} - x_j\|.$$

Setting

$$E_j = \int_0^1 G(x_j - t \sigma_j s_j) dt - G$$

we have again by Taylor's theorem

$$\begin{aligned}
g_{j+1} &= g_j - \sigma_j G s_j - \sigma_j E_j s_j \\
&= g_j - G s_j + (1 - \sigma_j) G s_j - \sigma_j E_j s_j
\end{aligned}$$

and

$$\begin{aligned}
\frac{\|g_{j+1}\|}{\|g_j\|} &\leq \frac{\|g_j - G s_j\|}{\|g_j\|} + |1 - \sigma_j| \frac{\|G s_j\|}{\|g_j\|} + \|E_j\| \frac{\|\sigma_j s_j\|}{\|g_j\|} \\
&= \frac{\|\rho_j g_j - G p_j\|}{\rho_j \|g_j\|} + |1 - \sigma_j| \frac{\|G p_j\|}{\rho_j \|g_j\|} + \|E_j\| \frac{\|\sigma_j s_j\|}{\|g_j\|}.
\end{aligned}$$

Since  $\|G p_j\| \geq \mu$  we obtain from Lemma 3, that for  $\gamma$  sufficiently small

$$\|\rho_j g_j - G p_j\| = O(\sqrt{\psi_j - 2}) \text{ and } \|\rho_j g_j\| \geq 0.5\mu.$$

Furthermore, by (5.2)

$$\frac{\|\sigma_j s_j\|}{\|g_j\|} \leq \frac{\|s_j\|}{\|g_j\|} \frac{\|g_j\| \|s_j\|}{\mu \|s_j\|^2} \leq \frac{1}{\mu}$$

and by (2.4),

$$\begin{aligned}
\|E_j\| &\leq \left\| \int_0^1 G(x_j - t \sigma_j s_j) dt - G_j \right\| + \|G_j - G\| \\
&\leq \max_{0 \leq t \leq 1} \{ \|G(x_j - t \sigma_j s_j) - G_j\| + \|G_j - G\| \} \\
&\leq L \|x_{j+1} - x_j\| + L \|x_j - z\| = O(\max\{\|g_j\|, \|g_{j+1}\|\}).
\end{aligned}$$

Therefore we have

$$\frac{\|g_{j+1}\|}{\|g_j\|} = O(\max\{\sqrt{\psi_j - 2}, \|g_j\|, \|g_{j+1}\|\}).$$

Theorem 3.

Let the sequences  $\{\sigma_j\}$ ,  $\{g_j\}$  and  $\{x_j\}$  be generated by the algorithm. Then

- i)  $|\sigma_j - 1| \rightarrow 0$  as  $j \rightarrow \infty$
- ii)  $\frac{\|g_{j+1}\|}{\|g_j\|} \rightarrow 0$  as  $j \rightarrow \infty$
- iii)  $\frac{\|x_{j+1} - z\|}{\|x_j - z\|} \rightarrow 0$  as  $j \rightarrow \infty$ .

Proof:

By Theorem 2,  $\|g_j\| \rightarrow 0$  as  $j \rightarrow \infty$ . If  $\tau_j \rightarrow 2$  as  $j \rightarrow \infty$ , it follows from Lemma 4 that  $\psi_j \rightarrow 2$ , which by Lemma 5 and (2.4) implies the statements of the theorem. Thus it suffices to show that

$$\tau_j \rightarrow 2 \text{ as } j \rightarrow \infty.$$

Since  $\tau_j \geq 2$  this is equivalent with proving that for every  $\epsilon > 0$  there is  $j(\epsilon)$  such that

$$\tau_j \leq 2 + \epsilon \text{ for } j \geq j(\epsilon).$$

Since  $\|d_j - Gp_j\| \rightarrow 0$  as  $j \rightarrow \infty$ , it follows from Lemma 3, that for  $j$  sufficiently large,

$$(5.3) \quad \begin{aligned} \omega_j &= 2 + O(\|d_j - Gp_j\|) \\ &= 2 + O(\max\{ \|g_j\|, \|g_{j+1}\| \}). \end{aligned}$$

Therefore, by (5.1)

$$\varphi_{j+1} = \varphi_j - \tau_j + 2 + O(\max\{ \|g_j\|, \|g_{j+1}\| \}).$$

Let

$$J = \{ j \mid \tau_j > 2 + \varepsilon \}.$$

Since  $\|g_j\| \rightarrow 0$  as  $j \rightarrow \infty$ , there is  $j_1$  such that

$$(5.4) \quad \begin{aligned} \varphi_{j+1} &\leq \varphi_j - (2 + \varepsilon) + 2 + O(\max\{ \|g_j\|, \|g_{j+1}\| \}) \\ &\leq \varphi_j - \frac{\varepsilon}{2} \quad \text{for } j \geq j_1 \quad \text{and } j \in J. \end{aligned}$$

If  $j \notin J$  and  $\varepsilon$  is sufficiently small it follows from Lemma 4 and 5 that there

is  $j_2$  such that

$$(5.5) \quad \|g_{j+2}\| \leq 0.5\|g_{j+1}\| \quad \text{for } j \geq j_2 \quad \text{and } j \notin J.$$

Thus, if  $j-1 \in J$ ,  $j+i \notin J$ ,  $i = 0, \dots, k-1$ ,  $j+k \in J$  it follows from (5.3)

and (5.5) that for  $j \geq j_2$

$$(5.6) \quad \begin{aligned} \varphi_{j+k} - \varphi_j &= (\varphi_{j+1} - \varphi_j) + (\varphi_{j+2} - \varphi_{j+1}) + \dots + (\varphi_{j+k} - \varphi_{j+k-1}) \\ &= O(\|g_j\|) + O(\|g_{j+1}\|) + \dots + O(\|g_{j+k-1}\|) \\ &= O(\|g_j\|) + O(2\|g_{j+1}\|). \\ &\leq \frac{\varepsilon}{4} \quad \text{for } j \text{ sufficiently large.} \end{aligned}$$

Since  $\varphi_j > 0$ , (5.4) and (5.6) imply that  $J$  has at most finitely many elements.

As a further application of (5.1) we obtain

Theorem 4.

The sequences

$$\{\|H_j\|\} \quad \text{and} \quad \{\|H_j^{-1}\|\}$$

are bounded.

Proof:

From (5.1) we have

$$\begin{aligned}\varphi_j &= \varphi_0 + \sum_{i=1}^{j-1} (\varphi_i - \varphi_{i-1}) \\ &= \varphi_0 + \sum_{i=1}^{j-1} (\omega_i - \tau_i) \\ &\leq \varphi_0 + \sum_{i=1}^{j-1} (\omega_i - 2)\end{aligned}$$

because  $2 - \tau_i \leq 0$  for all  $i$ . Since  $\|d_j - G p_j\| \rightarrow 0$  as  $j \rightarrow \infty$  it

follows from Lemma 3 that

$$\sum_{i=1}^{j-1} (\omega_i - 2) = O\left(\sum_{i=1}^{j-1} \|g_i\|^2\right) = O\left(\sum_{i=1}^{\infty} \|g_i\|^2\right) < \infty.$$

Thus the sequence  $\{\varphi_j\}$  is bounded. Moreover, in the proof of the previous theorem it has been shown that  $\tau_i \rightarrow 2$  as  $j \rightarrow \infty$ . Thus Lemma 4 implies that  $\psi_i \rightarrow 2$  as  $j \rightarrow \infty$ . Therefore

$$0 < \text{tr}(G^{\frac{1}{2}} H_j G^{\frac{1}{2}}) \leq \text{tr}(G^{-\frac{1}{2}} H_j^{-1} G^{-\frac{1}{2}}) = \varphi_j + \psi_j$$

is bounded. Since the trace of a matrix is equal to the sum of its eigenvalues, this means that there is a uniform upper bound for the eigenvalues of the matrices  $G^{\frac{1}{2}} H_j G^{\frac{1}{2}}$  and  $G^{-\frac{1}{2}} H_j^{-1} G^{-\frac{1}{2}}$ ,  $j = 0, 1, 2, \dots$ . Thus there is a uniform upper bound for the numbers  $\|H_j\|$  and  $\|H_j^{-1}\|$ ,  $j = 0, 1, 2, \dots$ .

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